ROTATIONAL SPECTRUM OF SACCHARINE

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A significant step forward in the structure-activity relationships of sweeteners was the assignment of the AH-B moiety in sweeteners by Shallenberger and Acree [a,b]. They proposed that all sweeteners contain an AH-B moiety, known as glucophore, in which A and B are electronegative atoms separated by a distance between 2.5 to 4 Å. H is a hydrogen atom attached to one of the electronegative atom by a covalent bond. For saccharine, one of the oldest artificial sweeteners widely used in food and drinks, two possible B moieties exist ,the carbonyl oxygen atom and the sulfoxide oxygen atom although there is a consensus of opinion among scientists over the assignment of AH-B moieties to HN-SO. In the present work, the solid of saccharine (m.p. 220^{o}C) has been vaporized by laser ablation (LA) and its rotational spectrum has been analyzed by broadband CP-FTMW and narrowband MB-FTMW Fourier transform microwave techniques. The detailed structural information extracted from the rotational constants and ^{14}N nuclear quadrupole coupling constants provided enough information to ascribe the glucophore's AH and B sites of saccharine.

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[a] R. S. Shallenberger, T. E. Acree. Nature 216, 480-482 Nov 1967.
[b] R. S. Shallenberger. Taste Chemistry; Blackie Academic & Professional, London, (1993).